

# **AEROSOL FORECAST OVER THE GREAT LAKES FOR A FEBRUARY 2005 EPISODE**

Pius Lee, Jeffery McQueen, Marina Tsidulko, Mary Hart, Shobha Kondragunta, Daiwen Kang, Geoff DiMego and Paula Davidson\*

## **1. INTRODUCTION**

Many local health and air quality agencies in the Upper Midwest and the Great Lakes regions had issued air advisories between January 31<sup>st</sup> and February 4<sup>th</sup>, 2005. Air Quality Index (AQI) values issued on the EPA web site for Minnesota peaked at 155 on January 31<sup>st</sup>. In the Chicago area, the AQI measured between 110 and 140 for most of the first week of February. The deterioration of air quality over these regions for a rather prolonged period has been attributed to the slow passing of broad high pressure systems centered over the Great Lakes. The pressure systems were accompanied by extensive cloudiness and snow cover over the same regions. This combination of meteorological conditions resulted in reduced atmospheric mixing; and high rates of atmospheric particle formation and growth due to high RH in the lower levels.

In this study, the National Weather Service (NWS) Eta meteorological model (Rogers et al. 1996) coupled with EPA Community Multiscale Air Quality model (CMAQ) (Byun and Ching 1999, Byun and Schere 2006) in the Air Quality Forecast Capability (AQFC) (Otte et al. 2005, Davidson et al. 2004) was used in a research mode to predict aerosol concentration and speciation of this poor air episode. The model result has been verified

---

\* Pius C. Lee<sup>#</sup>, Jeff McQueen<sup>@</sup>, Marina Tsidulko<sup>#</sup>, Mary Hart<sup>#</sup>, Shobha Kondragunta<sup>\$</sup>, Daiwen Kang<sup>~</sup>, Geoff DiMego<sup>@</sup>, and Paula Davidson<sup>+</sup>. <sup>#</sup>Scientific Applications International Corporation, Beltsville, MD, USA, <sup>@</sup>Environmental Modeling Center, National Centers for Environmental Prediction, NWS, MD, USA. <sup>\$</sup>National Environmental Satellite and Data Information Service, Camp Springs, MD, USA. <sup>~</sup>Science and Technology Corp., RTP, NC, USA. <sup>+</sup>Office of Science and Technology, NWS, Silver Spring, MD USA.

in a qualitative manner by comparing its Aerosol Optical Depth (AOD) prediction with that observed by the Geostationary Operational Environmental Satellites (GOES) (NOAA 2005a-b), and the surface level aerosol concentration prediction with that compiled by the Aerometric Information Retrieval Now (AIRNOW) (EPA 2005) observation network.

## 2. DERIVING PM<sub>2.5</sub> AND AOD

The aerosol module in CMAQ adopts a modal approach to represent the particles suspended in air (Binkowski and Roselle 2003; Mebust et al. 2003). It uses the superposition of 3 log-normal sub-distributions to represent the size distribution of these particles. Fine particles with a diameter less than 2.5  $\mu\text{m}$  (PM<sub>2.5</sub>) are represented by two of these sub-distributions called the Aitken (i mode) for particles with diameters up to 0.1  $\mu\text{m}$ , and the accumulation (j mode) for particles with diameters between 0.1 and 2.5  $\mu\text{m}$ . Table 1 shows a partial listing of the speciation of the particles in the i and j modes.

Table 1. A partial list of speciation and variable names used in the aerosol module

Species	Aitken mode	Accumulation mode
Sulfate	ASO4I	ASO4J
Ammonium	ANH4I	ANH4J
Nitrate	ANO3I	ANO3J
Anthropogenic secondary organic	AORGAi	AORGAJ
Primary organic mass	AORGPai	AORGPaj
Secondary biogenic organic mass	AORGBi	AORGBJ
Elemental carbon mass	ACEI	ACEJ
Unspecified anthropogenic mass	A25I	A25J
Water mass	AH2OI	AH2OJ

In this version of the model, coarse mode (diameter 2.5  $\mu\text{m}$  and greater) simulation are not included due to the large uncertainty in the determination of coarse particle emissions. Furthermore, in terms of health hazard considerations the effects caused by the two finer modes are of the most concern. By the same token, the model does not include coarse mode particles in its visual range calculations in terms of AOD.

In the model, PM<sub>2.5</sub> concentration in the surface level is derived by summing up all the concentrations pertaining to the species listed in Table 1. AOD, a dimensionless quantification of visibility impairment, is defined in the following equation:

$$AOD = \int_0^{ModelTop} B_{sp} dz \quad (1)$$

where  $B_{sp}$  is the aerosol extinction coefficient in  $\text{km}^{-1}$  and  $z$  is altitude in km.

CMAQ calculates  $B_{sp}$  using  $Q_{ext}$ , the extinction efficiency, a measure of light scattering efficiency which in turn is estimated using approximations to the Mie theory (Binkowski, 1999).

$$B_{sp} = \frac{3p}{2I} \int_{-\infty}^{\infty} \frac{Q_{ext}}{a} \frac{dV}{d \ln a} d \ln a \quad (2)$$

where  $a = \pi D^2/4$ ,  $D$  is the particle diameter,  $V$  is the volume of the particle, and  $I$  is the wavelength of the incident light.

### 3. METEOROLOGY OF JANUARY 31 & FEBRUARY 1, 2005

On both January 31<sup>st</sup> and February 1<sup>st</sup>, 2005, moderate to weak high pressure systems dominated much of the continental US as shown in Figs. 1a and 1b. There were essentially three large high pressure systems that together covered much of the middle to northern parts of the continental US. The high pressure system in the middle, located over the Midwest and Great Lakes, was the weakest and the fastest moving of the systems. In contrast with the other stronger systems on either side, which happened to be more stationary, this middle system experienced more cloudiness as it passed southward. The weak pressure gradients and generally fair weather conditions there rendered the air mass calm and stagnant. Satellite images on those days verified the cloudiness over the Midwest.

Over the Upper Midwest and Great Lakes, snow cover was prevalent and the surface level air temperature in those areas varied between -5°C and 5°C during the period. These temperatures and the abundance of water vapor resulting from the melting and sublimating snow provided a favorable condition for fog and hygroscopic aerosol growth. Consequently, low clouds and fog further inhibited mixing activities in the lower atmosphere. This compound condition of stagnant air, low cloud and rather warm temperatures around the freezing point gave rise to a heavy suspension of fog and aerosol particles in the lower atmosphere in the area for a prolonged period of time.

### 4. VERIFICATION OF AOD AND PM2.5

Figures 2b and 3b show the model predicted AOD and surface level PM2.5 concentrations. The shaded fields, using the side color bar color code, depict the dimensionless AOD values. They were obtained by evaluating Equations (2) and (1) through the use of predicted instantaneous aerosol concentrations. The colored line contours depict PM2.5 concentrations in  $\mu\text{g m}^{-3}$ .

To evaluate the model predicted AOD against observations we used AOD values retrieved from GOES satellites imagery. The time resolution of the satellite data retrieval is 30 minutes. Cloudiness can, however, deprive us of the opportunity for AOD data retrieval.

Figures 2b and 3b show high predicted values of AOD in the upper Midwest for the afternoons of both January 31<sup>st</sup> and February 1<sup>st</sup>, 2005 respectively. Figure 2b shows high predicted values of AOD around southeastern Louisiana on January 31<sup>st</sup>. Nonetheless, all these aforementioned areas were under clouds for most of time, preventing retrieval of AOD observation data from the GOES satellites. For the clear sky areas shown on the satellite imagery in Fig. 2c for January 31<sup>st</sup>, such as areas along the U.S. Eastern

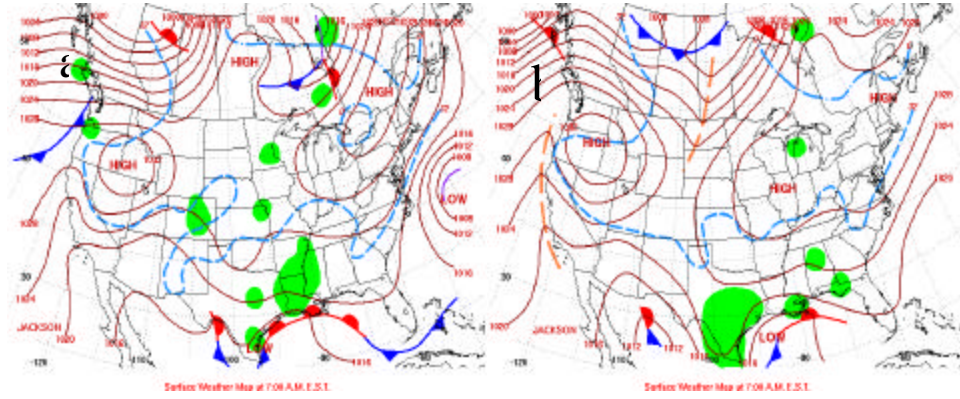


Figure 1: Surface weather map: (a) for January 31<sup>st</sup> and (b) for February 1<sup>st</sup> 2005.

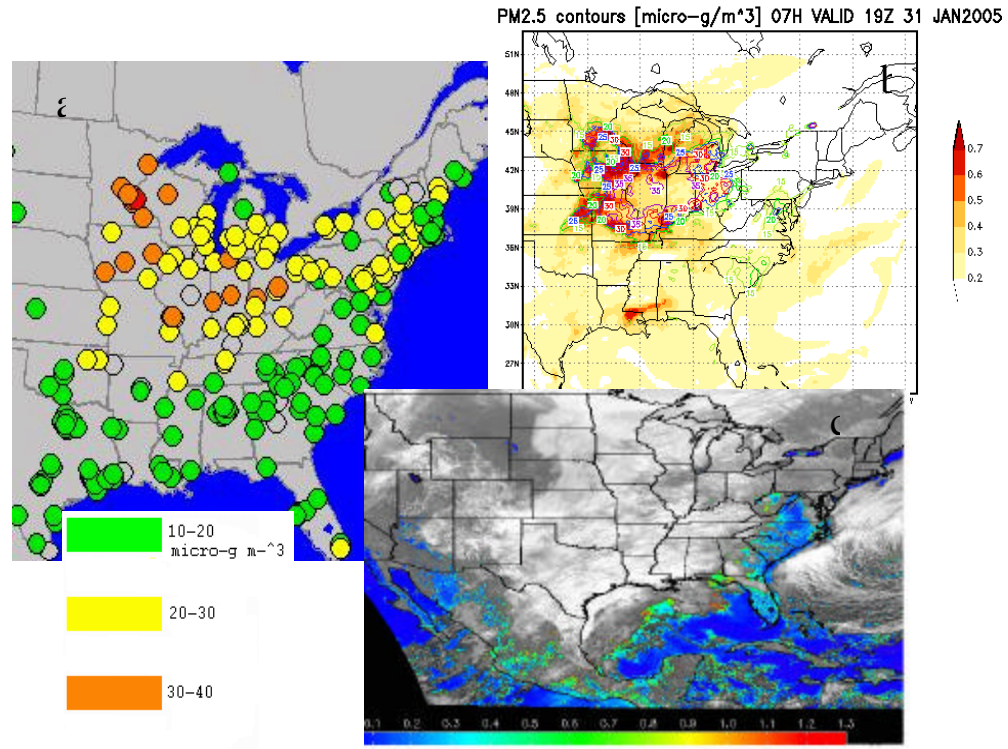


Figure 2: Predicted and observed column total AOD and surface level PM2.5 values valid at approximately 19 UTC January 31<sup>st</sup>, 2005: (a) Observed PM2.5 compiled by the AIRNOW network where green, yellow and orange data points represent concentration between, 10 and 20; 20 and 30; and 30 and 40  $\mu\text{g m}^{-3}$ , respectively, (b) predicted column total AOD, color shaded in accordance with the side color bar; and PM2.5, colored contour lines with labels: light green for 15, dark green for 20, blue for 25, red for 30, and

purple for  $35 \mu\text{g m}^{-3}$  respectively, and (c) GOES imagery showing clouds, along with retrieved AOD values.

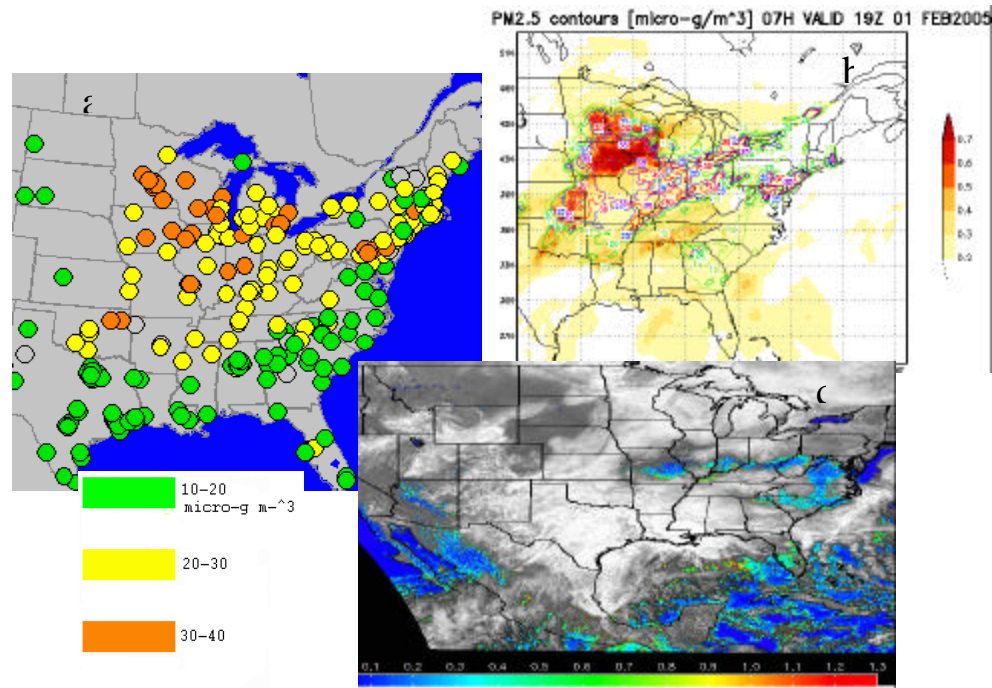


Figure 3: Equivalent to Fig. 2, but for February 1<sup>st</sup>, 2005.

Seaboard, the observed AOD ranged between 0.2 and 0.3, while there were a few sporadic high values above 1.0. They agreed rather well with those model predicted values shown in the corresponding areas in Fig. 2b. However, agreement in the high observed AOD values offshore of the Florida Panhandle is not good, as is shown in Figs. 2b and 2c. On February 1<sup>st</sup>, this agreement offshore of the Florida Panhandle improved as shown in Figs. 3b and 3c. There was a belt of clear sky extending from the middle of Missouri to Northern Virginia which looped around to northeastern Georgia. The observed and predicted AOD agreed quite well within this sunny stretch on the afternoon of February 1<sup>st</sup> as is shown in Figs. 2b and 2c.

Predicted surface PM2.5 aerosol concentrations, have been evaluated with the AIRNOW compiled observation data for the selected days as shown in Figs. 2a and 3a. Figure 2b shows a cluster of high predicted surface PM2.5 concentrations equal to or larger than 35  $\mu\text{gm}^{-3}$  for most of Ohio and Indiana on January 31<sup>st</sup>. It also shows 2 contour ‘tongues’ of values between 30 - 35  $\mu\text{gm}^{-3}$  extending from these states into southern Michigan and eastern Minnesota, respectively. The concentration levels of 15 - 20  $\mu\text{gm}^{-3}$  are shown along the U.S. Eastern Seaboard in Fig. 2b. These features were roughly apparent in the AIRNOW observations as shown in Fig. 2a.

For the afternoon of February 1<sup>st</sup>, the model predicted a cluster of high surface PM2.5 concentrations equal to or larger than 35  $\mu\text{gm}^{-3}$  expanding from the Upper Midwest southwards, reaching northern Oklahoma as shown in Fig. 3b. The figure also shows that

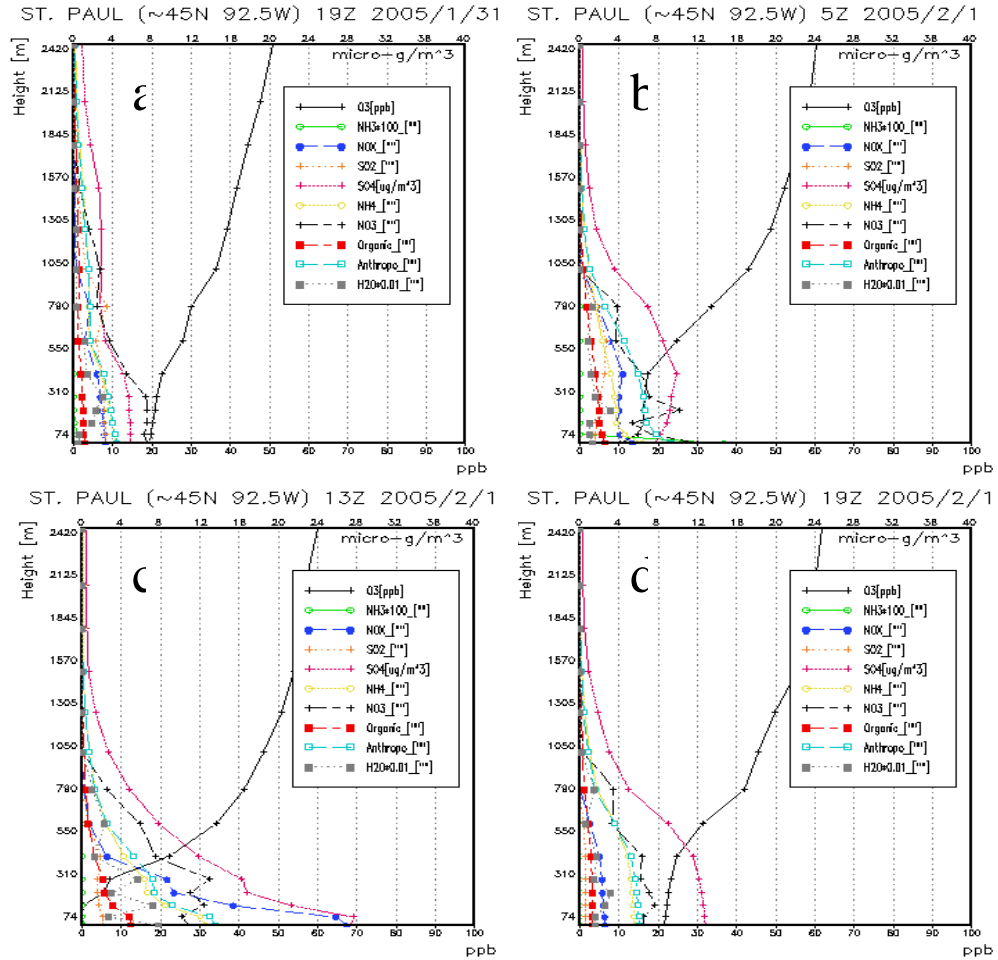


Figure 4: Predicted vertical concentration profiles at St. Paul, MN, for the following species:  $O_3$ ,  $NH_3$  (magnified 100 times),  $NO_x$ , and  $SO_2$ , all in ppb; and for aerosol species in  $\mu g m^{-3}$ :  $SO_4^{2-}$ ,  $NH_4^+$ ,  $NO_3^-$ , organic, anthropogenic, and water content at (a) 19 UTC January 31<sup>st</sup>, (b) 5 UTC February 1<sup>st</sup>, (c) 13z February 1<sup>st</sup>, and (d) 19 UTC February 1<sup>st</sup>, 2005.

the concentration level in the Boston-Philadelphia corridor increased to 30 - 35  $\mu g m^{-3}$ . These two features are evident in the AIRNOW observations as shown in Fig. 3a.

## 5. SPECIATION AND VERTICAL DISTRIBUTIONS

Knowledge about the speciation and spatial distribution of aerosols are key to understanding how well the PM concentrations are predicted. However, observations of these properties are not commonly available. Intense field campaigns help to provide data with dense spatial and temporal coverage during the campaign; in addition, there are a limited number of surface monitoring stations providing archival information on

speciation. The U.S. EPA is purposefully working to expand the capability of the AIRNOW network to provide vertical concentration profiles of major gaseous and particulate pollutants within the planetary boundary of the Continental US.

In this study, the surface PM2.5 concentration compiled by AIRNOW have been the primary verification data used, as shown in Figs. 2a and 3a. A brief examination of predicted concentration profiles of component aerosol species at two locations (St Paul and Chicago) serves to suggest some possible explanation of differences in surface level concentration of total PM2.5.

The model predicted that  $\text{SO}_4^{2-}$  and  $\text{NO}_3^-$  were the dominant species at the surface in regions of high PM2.5 concentration during the test period. Predicted high surface level concentrations of anthropogenic mass, primarily resulted from non-organic un-speciated emissions, shown in Figs 4 and 5 further suggest that anthropogenic sources played a major role in the episode.

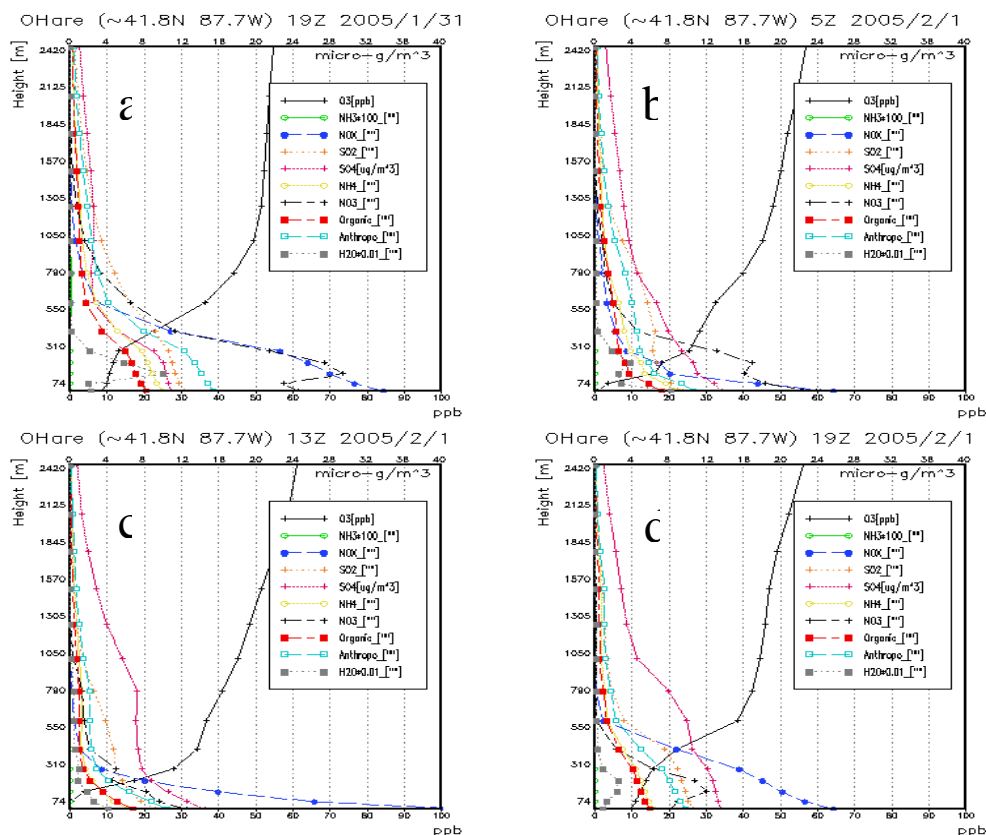


Figure 5: Equivalent to Fig. 4, but for O'Hare Airport, Chicago, IL.

Predicted vertical profiles of  $\text{NO}_x$  and  $\text{NO}_3^-$  follow one another closely as shown in Figs. 4 and 5. Similar precursor and product relationships are also reflected in  $\text{SO}_2$  and  $\text{SO}_4^{2-}$  concentrations. The profiles of  $\text{NH}_3$  and  $\text{NH}_4^+$  are, however, rather different, possibly reflecting the short life-time of the former relative to the latter.



Predicted vertical concentration profiles of O<sub>3</sub> and NO<sub>x</sub> almost always supplemented one another at all sites. This characteristic of the two species' profiles was especially noticeable at night and in the early morning when O<sub>3</sub> is titrated by NO<sub>x</sub>.

Predictions for the O'Hare site reflect high emissions of NO<sub>x</sub> as shown in Fig. 5. This NO<sub>x</sub>-rich air mass was probably due to heavier emissions from the transportation sector in the Chicago vicinity relative to St. Paul.

## 6. REFERENCES

- Binkowski, F. S. and S. J. Roselle, 2003: Models-3 Community Multiscale Air Quality (CMAQ) model aerosol component: 1: Model description, *J. Geophys. Res.*, 108(D6), 4183, doi:10.1029/2001JD001409.
- Binkowski, F. S., 1999: The aerosol portion of Models-3 CMAQ, in *Science Algorithm of the EPA Models-3 CMAQ Modeling System*, edited by D.W. Byun and J.K.S. Ching, Rep. EPA-600/R-99/030, pp 1-23.
- Byun, D. W., and J. K. S. Ching (Eds.), 1999: *Science algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System*. EPA-600/R-99/030, Office of Research and Development, U.S. Environmental Protection Agency, Washington, D.C. [Available from U.S. EPA, ORD, Washington, D.C. 20460.]
- Byun, D. W., and K. L. Schere, 2006: Description of the Models-3 Community Multiscale Air Quality (CMAQ) Model: System overview, governing equations, and science algorithms. *Appl. Mech. Rev.*, in press.
- Davidson, P. M., N. Seaman, K. Schere, R. A. Wayland, J. L. Hayes, and K. F. Carey, 2004: National air quality forecasting capability: First steps toward implementation. Preprints, *Sixth Conf. on Atmos. Chem.*, Amer. Met. Soc., Seattle, WA, 12-16 Jan 2004.
- EPA 2005: AIRNOW Network [Available at <http://www.epa.gov/airnow>]
- Mebust, M. R., B. K. Eder, F. S. Binkowski and S. J. Roselle, 2003: Models-3 Community Multiscale Air Quality (CMAQ) model aerosol component: 2: Model evaluation, *J. Geophys. Res.*, 108(D6), 4184, doi:10.1029/2001JD001410, 2003.
- NOAA, 2005a: National Environmental Satellite, GOES aerosol and SMOKE Product. [Available at <http://lwf.ncdc.noaa.gov/oa/climate/research/2005/fire05.html>]
- NOAA, 2005b: Satellite Service Division and Fire Detection Program. [Available at <http://www.ssd.noaa.gov/PS/FIRE/hms.html>]
- Otte, T.L., G. Pouliot, J. E. Pleim, J. O. Young, K. L. Schere, D. C. Wong, P. C. S. Lee, M. Tsidulko, J. T. McQueen, P. Davidson, R. Mathur, H.Y. Chuang, G. DiMego, and N. L. Seaman, 2005: Linking the Eta model with the Community Multiscale Air Quality (CMAQ) modeling system to build a national air quality forecasting system, *Wea. Forecasting*, 20 (No.3), 367-384.
- Rogers, E., T. Black, D. Deaven, G. DiMego, Q. Zhao, M. Baldwin, N. Junker, and Y. Lin, 1996: Changes to the operational "early" Eta Analysis / Forecast System at the National Centers for Environmental Prediction. *Wea. Forecasting*, 11, 391-413.

**Acknowledgements:** The authors appreciate numerous valuable discussions with Drs. Rohit Mathur, Jon Pleim, Tanya Otte, George Pouliot, Jeff Young, and Ken Schere of the Atmospheric Sciences Modeling Division of the Air Resources Laboratory at the National Oceanic and Atmospheric Administration office at Research Triangle Park, North Carolina. (They are currently on assignment to the National Exposure Research Laboratory, U.S. Environmental Protection Agency). The EPA AIRNOW program staff provided the observations necessary for quantitative model evaluation.

**Disclaimer:** The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number DW13921548. Although it has been reviewed by NOAA and approved for publication, it does not necessarily reflect its policies or views.